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=> file hcaplus
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FILE COVERS 1907 - 23 Mar 2007  VOL 146 ISS 14
FILE LAST UPDATED: 22 Mar 2007  (20070322/ED)

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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d que nos l32
L24          784 SEA FILE=HCAPLUS ABB=ON  PLU=ON  LARSEN, B?/AU
L25         1700 SEA FILE=HCAPLUS ABB=ON  PLU=ON  PETERSEN, J?/AU
L26          465 SEA FILE=HCAPLUS ABB=ON  PLU=ON  MEIER, E?/AU
L27            7 SEA FILE=HCAPLUS ABB=ON  PLU=ON  KJOLBYE, A?/AU
L28          171 SEA FILE=HCAPLUS ABB=ON  PLU=ON  JORGENSEN, N?/AU
L29         1501 SEA FILE=HCAPLUS ABB=ON  PLU=ON  NIELSEN, M?/AU
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L31          735 SEA FILE=HCAPLUS ABB=ON  PLU=ON  MARTINS, J?/AU
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                 L27 AND L28 AND L29 AND L30 AND L31
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Inventors Search

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=> d ibib ed abs l32 1-2

L32  ANSWER 1 OF 2  HCAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2002:754415  HCAPLUS  Full-text
DOCUMENT NUMBER:          137:263304
TITLE:                    Synthesis of peptides and medical uses of
                          intracellular communication facilitating
                          compounds
INVENTOR(S):              Larsen, Bjarne Due; Petersen,
                          Jorgen Soberg; Meier, Eddie;
                          Kjolbye, Anne Louise; Jorgensen,
                          Niklas Rye; Nielsen, Morten Schak
                          ; Holstein-Rathlou, Niels-Henrik;
                          Martins, James B.
PATENT ASSIGNEE(S):        Zealand Pharmaceuticals A/S, Den.
SOURCE:                   PCT Int. Appl., 233 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   2
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.        DATE
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WO 2002077017	A2	20021003	WO 2002-US5773	200202 22
WO 2002077017	A3	20031009		
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CA 2439101	A1	20021003	CA 2002-2439101	200202 22
EP 1370276	A2	20031217	EP 2002-723240	200202 22
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BR 2002007476	A	20060124	BR 2002-7476	200202 22
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US 2005113293	A1	20050526	US 2003-646294	200308 22
IN 2003DN01336	A	20050527	IN 2003-DN1336	200308 22
US 2005075280	A1	20050407	US 2004-772774	200402 04
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US 2001-314470P	P	200108 23
DK 2000-288	A	200002 23
DK 2000-738	A	200005 04
US 2000-251659P	P	200012 06
WO 2002-US5773	W	200202 22

OTHER SOURCE(S): MARPAT 137:263304
ED Entered STN: 04 Oct 2002
AB The invention relates to novel peptides, including novel antiarrhythmic peptides of linear or cyclic structure, having improved stability in vitro and/or in vivo, to compns. comprising these peptides, and to uses of the peptides for the preparation of medicaments. The invention also relates to the use of compds. that facilitate the intercellular communication for the preparation of medicaments for the treatment of a range of diseases characterized in impaired intercellular gap junctional communication. The invention further relates to a method of treating diseases, such as bladder incontinence, disorders of alveolar tissue and bronchial tissue, impaired hearing due to diseases of the cochlea, endothelial lesions, diabetic retinopathy and diabetic neuropathy, ischemia of the central nervous system and spinal cord, dental tissue disorders including periodontal disease, kidney diseases leading to hypertension, and a method of preventing failures of bone marrow transplantation. Ac-D-Tyr-D-Pro-D-4Hyp-Gly-D-Ala-Gly-NH2 (Hyp = hydroxyprolyl) was prepared by the solid-phase method and assayed for biol. activity. Graphs include those for relative cell-to-cell conductance, PI-turnover in neonatal rat cardiomyocytes, and ventricular APD90 dispersion.

L32 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:636085 HCAPLUS Full-text
DOCUMENT NUMBER: 135:180957
TITLE: Preparation of novel antiarrhythmic peptides
INVENTOR(S): Larsen, Bjarne Due; Petersen, Jorgen Soberg; Meier, Eddi; Kjolbye, Anne Louise; Jorgensen, Niklas Rye; Nielsen, Morten Schak ; Holstein-Rathlou, Niels-Henrik; Martins, James B.
PATENT ASSIGNEE(S): Zealand Pharmaceuticals A/S, Den.
SOURCE: PCT Int. Appl., 189 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001062775	A2	20010830	WO 2001-DK127	200102 22
WO 2001062775	A3	20020131		

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ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW

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CA 2385659 A1 20010830 CA 2001-2385659 200102 22

EP 1226160 A2 20020731 EP 2001-907393 200102 22

EP 1226160 B1 20041215

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JP 2003528826 T 20030930 JP 2001-562556 200102 22

AT 284896 T 20050115 AT 2001-907393 200102 22

ES 2228807 T3 20050416 ES 2001-1907393 200102 22

PT 1226160 T 20050429 PT 2001-907393 200102 22

AU 781674 B2 20050602 AU 2001-35362 200102 22

CA 2439101 A1 20021003 CA 2002-2439101 200202 22

WO 2002077017 A2 20021003 WO 2002-US5773 200202 22

WO 2002077017 A3 20031009

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW

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EP 1370276 A2 20031217 EP 2002-723240 200202 22

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JP 2005506295 T 20050303 JP 2002-576275 200202 22

BR 2002007476 A 20060124 BR 2002-7476 200202 22

NO 2003003641 A 20031020 NO 2003-3641 200308 15

US 2005113293 A1 20050526 US 2003-646294 200308 22

US 2005075280 A1 20050407 US 2004-772774

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PRIORITY APPLN. INFO.:			DK 2000-288	A	
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					200102 22
			WO 2001-DK127	W	
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			US 2001-314470P	P	
					200108 23
			WO 2002-US5773	W	
					200202 22

OTHER SOURCE(S): MARPAT 135:180957
ED Entered STN: 31 Aug 2001
AB Peptides X-A-B-Y and cyclo(X-A-B-Y) [A and B represents chemical moieties having an amino group (radical) and a carboxy group; X represents a peptide sequence of 1 to 3 D- or L-amino acid residues or an N-terminal modification of the group A-B when Y represents a C-terminal peptide sequence of 2 to 5 D- or L-amino acid residues; X represents a peptide sequence of 2 to 5 D- or L-amino acid residues when Y represents a C-terminal peptide sequence of 1 to 3 D- or L-amino acid residues; for the linear peptide, X is optionally chemical modified at its N-terminal and has an optional linking group comprising 0-8 backbone atoms] and their mirror image or a retro analogs or pharmaceutically acceptable derivs. were prepared for treating cardiac arrhythmias. Thus, Ac-D-Tyr-D-pro-D-4Hyp-Gly-D-Ala- Gly-NH2 (4Hyp = 4-hydroxyprolyl) was prepared by the solid-phase method using TentaGel-S-Ram and examined for biol. activity [assays included effect on gap junction intercellular communication (GJIC) in cardiomyocytes, binding to tissue prepns. of murine heart, and effect on cAMP formation in CHO cells].

=> file reg
FILE 'REGISTRY' ENTERED AT 17:47:15 ON 23 MAR 2007
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STRUCTURE FILE UPDATES: 22 MAR 2007 HIGHEST RN 927959-98-6
DICTIONARY FILE UPDATES: 22 MAR 2007 HIGHEST RN 927959-98-6

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http://www.cas.org/ONLINE/UG/regprops.html

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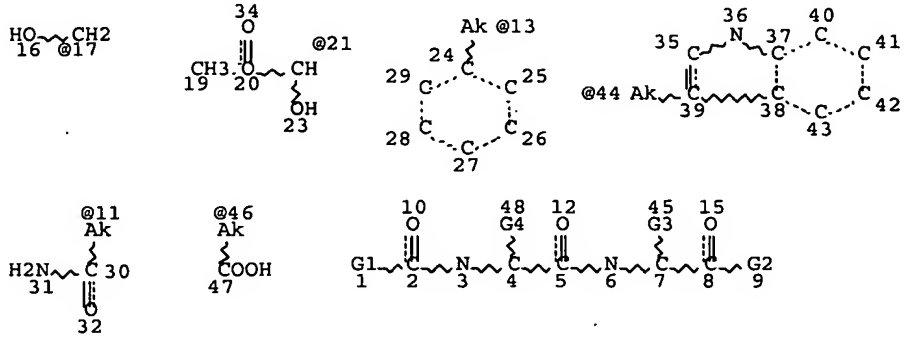
L20 STR



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GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
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STEREO ATTRIBUTES: NONE
L22 15 SEA FILE=REGISTRY SSS FUL L20

100.0% PROCESSED 859694 ITERATIONS 15 ANSWERS
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FILE COVERS 1907 - 23 Mar 2007 VOL 146 ISS 14
FILE LAST UPDATED: 22 Mar 2007 (20070322/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d que nos l23
L20 STR
L22 15 SEA FILE=REGISTRY SSS FUL L20
L23 19 SEA FILE=HCAPLUS ABB=ON PLU=ON L22

Structure Search

L23 ANSWER 1 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:61250 HCAPLUS Full-text
DOCUMENT NUMBER: 146:143006
TITLE: Preparation of N- or C-terminally modified small peptides for pharmaceutical use
INVENTOR(S): Larsen, Bjarne Due; Kerns, Edward H.
PATENT ASSIGNEE(S): Zealand Pharma A/S, Den.; Kiddle, Simon John
SOURCE: PCT Int. Appl., 54pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007007060	A2	20070118	WO 2006-GB2527	200607 07

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.:	GB 2005-14071	A	200507 07
	US 2005-697138P	P	200507 07

OTHER SOURCE(S): MARPAT 146:143006
ED Entered STN: 19 Jan 2007

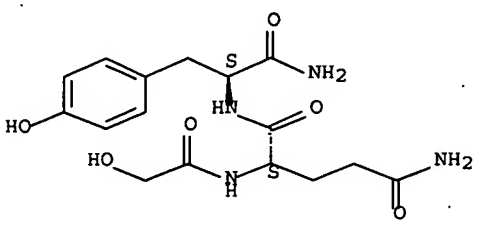
AB The invention discloses N- or C-terminally modified small peptides having antiarrhythmic and improved pharmacokinetic properties and a reduced tendency to inhibit the activity of isoenzyme 3A4 of cytochrome P 450 oxidase. Thus, N-(hydroxyacetyl)-Gly-Tyr-NH2 was prepared by the solid-phase method and shown to exhibit antiarrhythmic activity (48.7% response in the calcium-induced arrhythmia assay).

IT 919104-63-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N- or C-terminally modified small peptides having antiarrhythmic activity)

RN 919104-63-5 HCAPLUS

CN L-Tyrosinamide, N2-(2-hydroxyacetyl)-L-glutaminyl- (CA INDEX NAME)

Absolute stereochemistry.



L23 ANSWER 2 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:1130891 HCAPLUS Full-text

DOCUMENT NUMBER: 143:399818

TITLE: CD23-binding peptides and peptidomimetics for treatment of autoimmune and inflammatory disorders

INVENTOR(S): Mossalayi, Mohammad Djavad; Moynet, Daniel; Vincendeau, Philippe; Rambert, Jerome; Self, Christopher R.

PATENT ASSIGNEE(S): Universite Bordeaux 2, Fr.

SOURCE: PCT Int. Appl., 59 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005098435	A2	20051020	WO 2005-IB1133	20050405
WO 2005098435	A3	20060330		

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AU 2005229779	A1	20051020	AU 2005-229779	200504

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CA 2560726	A1	20051020	CA 2005-2560726	200504 05
EP 1733231	A2	20061220	EP 2005-718527	200504 05

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR

PRIORITY APPLN. INFO.:	EP 2004-290899	A 200404 05
	WO 2005-IB1133	W 200504 05

OTHER SOURCE(S): MARPAT 143:399818

ED Entered STN: 21 Oct 2005

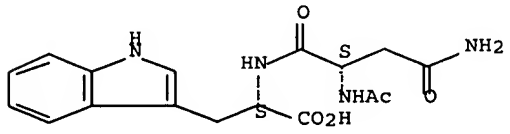
AB The invention describes compds. comprising new and useful peptides and peptidomimetics that can bind to CD23. They are capable of reducing inflammatory responses associated with auto-immune diseases, chronic inflammatory diseases, allergies and other inflammatory conditions such as those mediated by the mammalian immune system. Compds. of the invention relate to a CD23-binding peptide wherein said peptide comprises an amino-acid sequence of X1-X2- X3-X4-X5-X6-X7-X8, wherein: X1 is Phe, or is absent; X2 is His or Ala; X3 is Glu, Ser, Ala, Asn, Lys, or Cys; X4 is Asn, Phe, Gln, Pro, Ser, or Ala; X5 is Trp; X6 is Pro, Arg, Glu, Gly, Cys, or Lys; X7 is Ser, Pro, Leu, Thr Ala, Gly, Asn, or absent; and X8 is Phe, Gly, or is absent. Treatment of arthritic rats with peptide p30A resulted in remission of the arthritic condition and produced weight gain.

IT 867069-28-1P 867069-48-5P
RL: BPN (Biosynthetic preparation); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(CD23-binding peptides and peptidomimetics for treatment of autoimmune and inflammatory disorders)

RN 867069-28-1 HCAPLUS

CN L-Tryptophan, N2-acetyl-L-asparaginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 867069-48-5 HCAPLUS

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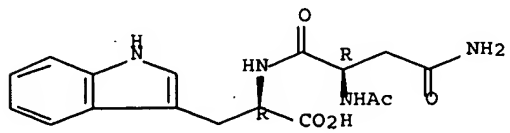
Absolute stereochemistry.

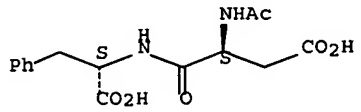


L23 ANSWER 3 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:1025958 HCAPLUS Full-text

DOCUMENT NUMBER: 142:477847
TITLE: Aspartame and aspartame derivatives effect human thrombin catalytic activity
AUTHOR(S): Scheffler, Julie E.; Berliner, Lawrence J.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Denver, Denver, CO, 80208-2436, USA
SOURCE: Biophysical Chemistry (2004), 112(2-3), 285-291
CODEN: BICIAZ; ISSN: 0301-4622
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:477847
ED Entered STN: 30 Nov 2004
AB The study of small Asp-Phe analogs was undertaken since this dipeptide sequence is critical in fibrinogen recognition and catalysis. The inhibition of clotting activity by Asp-Phe-Me ester (aspartame), formyl-Asp-Phe-Me ester and acetyl-Asp-Phe was biphasic in all cases, indicating the presence of at least two binding sites. The N-terminally blocked derivs. are stronger inhibitors than aspartame. In contrast, tosyl-Gly-Pro-Arg-p'-nitroanilide hydrolysis was inhibited minimally by Asp-Phe-Me, ester [Ki(app)=98 mM]. Acetyl-Asp-Phe inhibition of thrombin amidase activity was biphasic, tenfold stronger and appeared to be strongly cooperative. These results are discussed with respect to the inhibition of α-thrombin by ATP.
IT 108274-49-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(aspartame and aspartame derivs. effect human thrombin catalytic activity)
RN 108274-49-3 HCAPLUS
CN L-Phenylalanine, N-(N-acetyl-L-α-aspartyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 4 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:982484 HCAPLUS Full-text
DOCUMENT NUMBER: 140:164220
TITLE: Tryptophan as a probe for acid-base equilibria in peptides
AUTHOR(S): Marquezin, Cassia Alessandra; Hirata, Izaura Yoshico; Juliano, Luiz; Ito, Amando Siuiti
CORPORATE SOURCE: Instituto de Fisica da Universidade de Sao Paulo, Brazil
SOURCE: Biopolymers (2003), 71(5), 569-576
CODEN: BIPMAA; ISSN: 0006-3525
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 17 Dec 2003
AB We present results of time resolved fluorescence measurements performed in Tryptophan (Trp) derivs. and Trp-containing peptides in the pH range 3.0-11.0. For each compound, a set of decay profiles measured in a given range of pH values was examined as a whole using the global anal. technique. The data were fitted to two or three lifetime components and the anal. allowed the monitoring of the changes in the concentration of the different species contributing to the total fluorescence in that pH interval. The decay components were sensitive to the ionization state of groups neighboring the

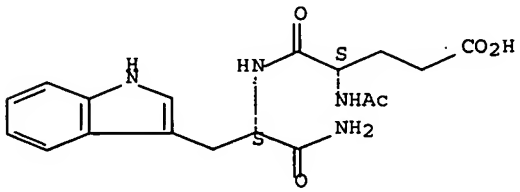
indole ring and pK values for the equilibrium between protonated and deprotonated species were obtained from the preexponential factor of the lifetime components. In Trp, protonation of the amino terminal of the rotamer having electron transfer rate comparable to fluorescence decay rates was responsible for the interconversion of a long lifetime component to the 2.9 ns component usually observed in neutral pH. Trp-X peptides also have a single rotamer dominating the decay that is quenched by NH3+. X-Trp peptides seem to be conformationally less restricted and it is possible that rotamer interconversion occur at high pH, increasing the population of nonquenched rotamers. Interconvertion between rotameric conformations of Trp are also present in the titration of ionizable groups in the side chain of peptides like His-Trp and Glu-Trp and control of pH is essential to the correct interpretation of fluorescence data in the study of peptides having such groups near to the Trp residue.

IT 656240-68-5
RL: PRP (Properties)
(tryptophan as probe for acid-base equilibrium in peptides)

RN 656240-68-5 HCAPLUS

CN L-Tryptophanamide, N-acetyl-L-α-glutamyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 5 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:283177 HCAPLUS Full-text

DOCUMENT NUMBER: 137:63466

TITLE: Quantitative structure-activity relationship: IX. Estimation of logP for some peptides

AUTHOR(S): Golovanov, I. B.; Tsygankova, I. G.

CORPORATE SOURCE: Institute of Theoretical and Experimental Biophysics, Russian Academy of Sciences, Pushchino, Russia

SOURCE: Russian Journal of General Chemistry (Translation of Zhurnal Obshchei Khimii) (2002), 72(1), 137-143
CODEN: RJGCEK; ISSN: 1070-3632

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 16 Apr 2002

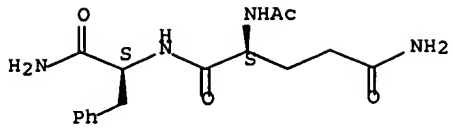
AB Based on the previously described quant. structure-activity relationship, estns. were made for the distribution factor (logP) in the octanol-water system of amides of N-acetyl peptides and peptides containing up to five amino acid residues. Data for di- and tripeptides reasonably agree with the available exptl. data.

IT 132765-93-6 132765-99-2
RL: PRP (Properties)
(quant. mol. structure-property relationship and calcn. of distribution factor for peptides in octanol-water system)

RN 132765-93-6 HCAPLUS

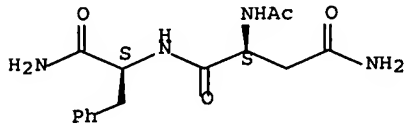
CN L-Phenylalaninamide, N2-acetyl-L-glutaminyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



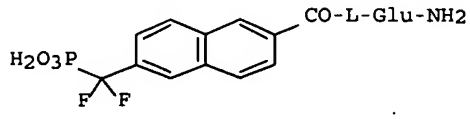
RN 132765-99-2 HCAPLUS
CN L-Phenylalaninamide, N2-acetyl-L-asparaginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

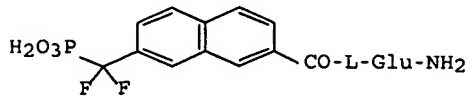


REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

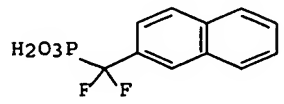
L23 ANSWER 6 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:737268 HCAPLUS Full-text
DOCUMENT NUMBER: 130:95825
TITLE: Structure-based design and synthesis of small molecule protein-tyrosine phosphatase 1B inhibitors
AUTHOR(S): Yao, Zhu-Jun; Ye, Bin; Wu, Xiong-Wu; Wang, Shaomeng; Wu, Li; Zhang, Zhong-Yin; Burke, Terrence R., Jr.
CORPORATE SOURCE: Laboratory of Medicinal Chemistry, Division of Basic Sciences, National Cancer Institute, National Institutes of Health, Bethesda, MD, 20892, USA
SOURCE: Bioorganic & Medicinal Chemistry (1998), 6(10), 1799-1810
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 20 Nov 1998
GI



I



II



III

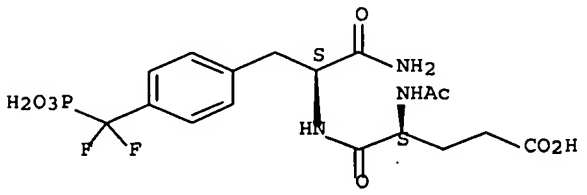
AB Protein-tyrosine phosphatase (PTP) inhibitors are attractive as potential signal transduction-directed therapeutics which may be useful in the treatment of a variety of diseases. New naphthyldifluoromethyl phosphonic acids I and II were designed bearing acidic functionality intended to interact with the protein-tyrosine phosphatase 1B (PTP1B) Arg47, which is situated just outside the catalytic pocket. This residue has been shown previously to provide key interactions with acidic residues of phosphotyrosyl-containing peptide substrates. Consistent with trends predicted by mol. dynamics calcns., the new analogs bound with 7- to 14-fold higher affinity than the parent III, in principal validating the design rationale.

IT 219316-38-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of glutamate-substituted naphthyldifluoromethylphsophonic acids as protein-tyrosine phosphatase 1B inhibitors)

RN 219316-38-8 HCAPLUS

CN L-Phenylalaninamide, N-acetyl-L-α-glutamyl-4-(difluorophosphonomethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

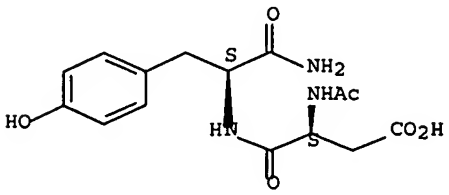
L23 ANSWER 7 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:89038 HCAPLUS Full-text
DOCUMENT NUMBER: 128:254233
TITLE: Correlation between binding and dynamics at SH2 domain interfaces
AUTHOR(S): Kay, Lewis E.; Muhandiram, D. R.; Wolf, Gert; Shoelson, Steven E.; Forman-Kay, Julie D.
CORPORATE SOURCE: Protein Engineering Network Centres Excellence, Departments Medical Genetics, Biochemistry, Chemistry, University Toronto, Toronto, ON, M5S 1A8, Can.
SOURCE: Nature Structural Biology (1998), 5(2), 156-163
CODEN: NSBIEW; ISSN: 1072-8368
PUBLISHER: Nature America
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 16 Feb 1998

AB Protein recognition is a key determinant in regulating biol. processes. Structures of complexes of interacting proteins provide significant insights into the mechanism of specific recognition. However, studies performed by modifying residues within a protein interface demonstrate that binding is not fully explained by these static pictures. Thus, structural data alone was not predictive of affinities in binding studies of phospholipase Cγ1 and Syp phosphatase SH2 domains with phosphopeptides. NMR relaxation expts. probing dynamics of Me groups of these complexes indicate a correlation between binding energy and restriction of motion at the interfacial region responsible for specific binding.

IT 205174-01-2
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process).
(correlation between binding and dynamics at SH2 domain

interfaces)
RN 205174-01-2 HCAPLUS
CN L-Tyrosinamide, N-acetyl-L-α-aspartyl- (9CI) (CA INDEX NAME)

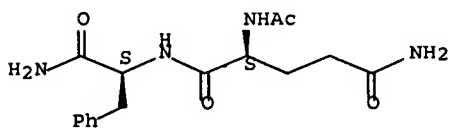
Absolute stereochemistry.



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

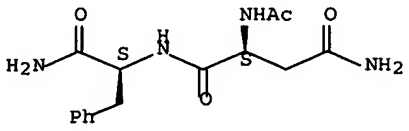
L23 ANSWER 8 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:34211 HCAPLUS Full-text
DOCUMENT NUMBER: 128:190087
TITLE: Octanol-water partition of nonzwitterionic peptides: predictive power of a molecular size-based model
AUTHOR(S): Buchwald, Peter; Bodor, Nicholas
CORPORATE SOURCE: Center for Drug Discovery, University of Florida, Health Science Center, Gainesville, FL, 32610-0497, USA
SOURCE: Proteins: Structure, Function, and Genetics (1998), 30(1), 86-99
CODEN: PSFGEY; ISSN: 0887-3585
PUBLISHER: Wiley-Liss, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 21 Jan 1998
AB A remarkably simple, mol. size-based model developed to predict octanol-water partition coeffs. for organic compds. is tested on a set of 188 neutral peptides with available exptl. partition data. Despite using only two parameters, it gives a promising correlation ($r^2 = 0.914$; $\sigma = 0.455$, $F = 1978.0$), and predictions are in a realistic range even for larger peptides (cyclosporin, melanotan, sandostatin) where common, overparametrized fragment methods become quite unreliable. Ion-pair partitioning and the extraction constant formalism is briefly reviewed to describe the sigmoidal lipophilicity profile of ionizable, nonzwitterionic peptides. It seems possible to extend the present model to estimate apparent partition coeffs. measured around neutral pH and physiol. conditions for monoionic peptides; however, as no standard conditions are yet defined and only relatively small number of exptl. data are available, the situation here is more complex.
IT 132765-93-6 132765-99-2
RL: PRP (Properties)
(octanol-water partition of nonzwitterionic peptides and predictive power of mol. size-based model)
RN 132765-93-6 HCAPLUS
CN L-Phenylalaninamide, N2-acetyl-L-glutaminyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 132765-99-2 HCAPLUS
CN L-Phenylalaninamide, N2-acetyl-L-asparaginyl- (9CI) (CA INDEX NAME)

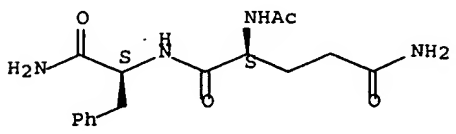
Absolute stereochemistry.



REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

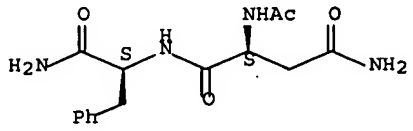
L23 ANSWER 9 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:977158 HCAPLUS Full-text
DOCUMENT NUMBER: 124:97406
TITLE: Hydrophobic contribution constants of amino acid residues to the hydrophobicities of oligopeptides
AUTHOR(S): Gao, Hua; Wang, Fengzhen; Lien, Eric, J.
CORPORATE SOURCE: Department Pharmaceutical Sciences, University Southern California, Los Angeles, CA, 90033, USA
SOURCE: Pharmaceutical Research (1995), 12(9), 1279-83
CODEN: PHREEB; ISSN: 0724-8741
PUBLISHER: Plenum
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 Dec 1995
AB The main purpose of this study is to explore the additive-constitutive nature of common amino acids in their contribution to the partition coeffs. of small peptides. The Log P values and other physico-chemical parameters of the peptides studied are taken from the literature. The frequency of appearance (ni) of each individual amino acid is calculated as the number of the amino acids in a given peptide. The partition coeffs. (Log P(oct./buff.) at pH 7) of 87 N-acetyl-peptide-amides have been correlated with the frequency of appearance of amino acids. From the correlation obtained, the de novo hydrophobic contribution consts. of 19 amino acid residues are derived for the first time. The contribution consts. are extended to 59 unmodified regular peptides with the inclusion of the pka values of both N-terminal and C-terminal amino acids. The models thus obtained have been validated with addnl. 27 peptides (both N-acetyl-peptide-amides and unmodified). The Log P of oligopeptides is very well correlated with the de novo hydrophobic contribution consts. of amino acids. The models we have derived are reasonably accurate in predicting the hydrophobicities of new oligopeptides (≤tetrapeptides) at a fixed pH (e.g., 7).
IT 132765-93-6 132765-99-2
RL: PRP (Properties)
(hydrophobic contribution consts. of amino acid residues to hydrophobicities of oligopeptides)
RN 132765-93-6 HCAPLUS
CN L-Phenylalaninamide, N2-acetyl-L-glutaminyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



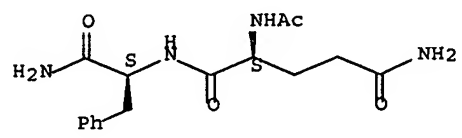
RN 132765-99-2 HCAPLUS
CN L-Phenylalaninamide, N2-acetyl-L-asparaginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



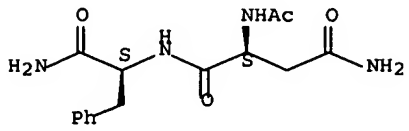
L23 ANSWER 10 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:11164 HCAPLUS Full-text
DOCUMENT NUMBER: 122:214479
TITLE: Quantitative Analyses of the Structure-Hydrophobicity Relationship for N-Acetyl Di- and Tripeptide Amides
AUTHOR(S): Akamatsu, Miki; Katayama, Takashi; Kishimoto, Daisuke; Kurokawa, Youichi; Shibata, Hiroyuki; Ueno, Tamio; Fujita, Toshio
CORPORATE SOURCE: Department of Agricultural Chemistry, Kyoto University, Kyoto, 606-01, Japan
SOURCE: Journal of Pharmaceutical Sciences (1994), 83(7), 1026-33
CODEN: JPMSAE; ISSN: 0022-3549
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 08 Nov 1994
AB The partition coefficient (P) of neutral species and the apparent partition ratio (P') at pH 7 of the ionized form were measured with the 1-octanol/water system for a number of N-acetyl di- and tripeptide amides having un-ionizable and ionizable side chains. Their log values were studied in terms of free-energy-related substituent and substructural parameters using regression anal. to give correlation equations of high quality physicochem. as well as statistically. The intrinsic hydrophobicity of side-chain substituents and their steric effect on the relative solvation of the backbone CONH groups were significant in determining the log P values of the un-ionizable acetyl peptide amides. For the log P value of peptides with polar side-chain substituents, resp. indicator variable terms were required to account for the sum of specific effects of substituents such as intramol. hydrogen-bond formation and the "polar proximity factor" for augmentation of the hydrophobicity. For the log P'(pH 7) value of basic and acidic peptides, the ability of counterionic species to form ion-pairs, the change in the apparent hydrophobicity of ionizable groups from the intrinsic value for their nonionized forms, the effect of ion-pairing itself, and other effects were addnl. considered. From the regression coeffs. of the parameter terms in correlation equations an effective hydrophobicity index was defined for each side chain, and the application and its limitation were suggested.
IT 132765-93-6 132765-99-2
RL: PRP (Properties)
(quant. anal. of the structure-hydrophobicity relationship for N-acetyl di- and tripeptide amides)
RN 132765-93-6 HCAPLUS
CN L-Phenylalaninamide, N2-acetyl-L-glutaminyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 132765-99-2 HCAPLUS
CN L-Phenylalaninamide, N2-acetyl-L-asparaginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

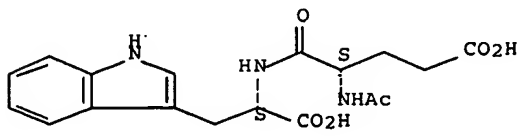


L23 ANSWER 11 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:415621 HCAPLUS Full-text
DOCUMENT NUMBER: 115:15621
TITLE: Infusion solutions containing N-acylated dipeptides and reducing sugars
INVENTOR(S): Kosegi, Koji; Tsukamoto, Yoshitsugu; Yaginuma, Hideya; Sato, Makoto; Amino, Mitsuto
PATENT ASSIGNEE(S): Morishita Pharmaceutical Co., Ltd., Japan; Ajinomoto Co., Inc.
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02286624	A	19901126	JP 1989-106946	19890425
PRIORITY APPLN. INFO.:			JP 1989-106946	19890425

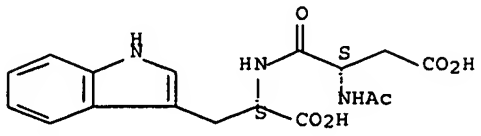
ED Entered STN: 12 Jul 1991
AB Infusion solns. contain reducing sugars and N-acylated dipeptides (C terminal = L-tryptophan residue). The dipeptides do not cause Mailard reaction or discoloration with the sugars, are stable in the solns., and show high bioavailability. Ratio of tryptophan formation in homogenized liver or kidney from N-acetyl-Ala-Trp (I) was much higher than from N-acetyl-Trp. An infusion solution was prepared from I, amino acids, glucose, AcOK, KH2PO4, MgSO4.7H2O, NaCl, and Ca gluconate.H2O.
IT 134321-04-3 134321-05-4
RL: BIOL (Biological study)
(infusion solns. containing glucose and)
RN 134321-04-3 HCAPLUS
CN L-Tryptophan, N-(N-acetyl-L-α-glutamyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



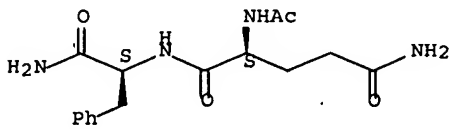
RN 134321-05-4 HCAPLUS
CN L-Tryptophan, N-(N-acetyl-L-α-aspartyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



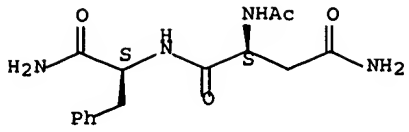
L23 ANSWER 12 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:143996 HCAPLUS Full-text
DOCUMENT NUMBER: 114:143996
TITLE: Hydrophobicity of N-acetyl-di- and tripeptide amides having unionizable side chains and correlation with substituent and structural parameters
AUTHOR(S): Akamatsu, Miki; Okutani, Shinichi; Nakao, Kazuya; Hong, Nam Joo; Fujita, Toshio
CORPORATE SOURCE: Dep. Agric. Chem., Kyoto Univ., Kyoto, 606, Japan
SOURCE: Quantitative Structure-Activity Relationships (1990), 9(3), 189-94
CODEN: QSARDI; ISSN: 0931-8771
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 19 Apr 1991
AB The log P value of 53 N-acetyldi- and -tripeptide amides composed of amino acids having unionizable side chains was measured in a 1-octanol/pH 7.0 aqueous buffer system. The factors governing the variations in the log P value among these protected peptides were quant. analyzed to formulate a correlation equation with free energy-related physicochem. and substructural parameters. The log P value was governed by the sum of the hydrophobicity of side chains and the backbone as well as by the steric effects of side chain substituents on the relative solvation of the backbone CONH groups. The log P value decreases by 0.6 log unit for the peptide bond, other factors being equal. For amino acids with polar side chains, the log P value was also affected by the polar proximity factor and intramol. hydrogen bond formation in a way similar to that of zwitterioonized peptides reported previously.
IT 132765-93-6 132765-99-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(partition coefficient and physicochem. parameters of)
RN 132765-93-6 HCAPLUS
CN L-Phenylalaninamide, N2-acetyl-L-glutaminyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



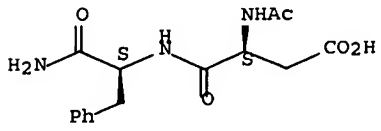
RN 132765-99-2 HCAPLUS
CN L-Phenylalaninamide, N2-acetyl-L-asparaginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L23 ANSWER 13 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:493824 HCAPLUS Full-text
DOCUMENT NUMBER: 113:93824
TITLE: Inhibition of chymotrypsin by peptidyl trifluoromethyl ketones: determinants of slow-binding kinetics
AUTHOR(S): Brady, Kenneth; Abeles, Robert H.
CORPORATE SOURCE: Dep. Toxicol., Harvard Sch. Public Health, Boston, MA, 02115, USA
SOURCE: Biochemistry (1990), 29(33), 7608-17
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 16 Sep 1990
AB A series of 7 peptidyl trifluoromethyl ketone (TFK) inhibitors of chymotrypsin were prepared which differ at the P1 and P2 subsites. Inhibition equilibrium and kinetics of association and dissociation with chymotrypsin were measured. The association rate of Ac-Phe-CF3 was measured at enzyme concns. between 8 nM and 117 μM in order to examine the relation between the ketone/hydrate equilibrium of trifluoromethyl ketones and the slow binding by these inhibitors. The association rate decreased at high enzyme concns., indicating that TFK ketone is the reactive species and that conversion of TFK hydrate to TFK ketone becomes rate limiting under these conditions. Inhibitors with hydrophobic side-chains at P2 bound more tightly but more slowly to chymotrypsin, indicating that formation of van der Waals contacts between the P2 side-chain and the histidine-57 and isoleucine-99 side-chains of chymotrypsin is a relatively slow process. Inhibitor properties were compared to the Michaelis-Menten kinetic consts. of a homologous series of peptide Me ester and peptide amide substrates. Plots of log Ki vs. log(kcat/Km) were linear with slopes of 0.65, indicating that these inhibitors are able to utilize 65% of the total binding energy between chymotrypsin and its hydrolytic transition state.
IT 128550-52-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 128550-52-7 HCAPLUS
CN L-Phenylalaninamide, N-acetyl-L-α-aspartyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L23 ANSWER 14 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:473918 HCAPLUS Full-text
DOCUMENT NUMBER: 109:73918
TITLE: Preparation of N-protected L-α-aspartyl-L-phenylalanines
INVENTOR(S): Takemoto, Tadashi; Hisamitsu, Kunio; Yugawa, Toshihide
PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62263197	A	19871116	JP 1986-104321	19860507
JP 06096595	B	19941130		
JP 07145193	A	19950606	JP 1994-112379	19940526
JP 2513159	B2	19960703		

PRIORITY APPLN. INFO.: JP 1986-104321 19860507

ED Entered STN: 02 Sep 1988

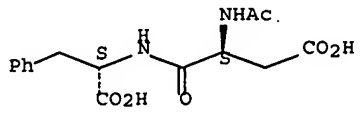
AB N-Protected L-α-aspartyl-L-phenylalanines, useful as intermediates for aspartame, were prepared by treating N-protected L-aspartic acid anhydride with L-phenyalanine in aqueous solvents at pH ≥ 7 in the presence of (in)organic acid salts of alkali metals or alkaline earth metals. Thus, N-formyl-L-aspartic acid anhydride was added to aqueous solution of L-phenylalanine Na salt monohydrate (I) in the presence of NaCl at -20° and pH 12.0-12.5 to give 73.5% N-formyl-L-α-aspartyl-L-phenylalanine (based on I).

IT 108274-49-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for aspartame)

RN 108274-49-3 HCAPLUS

CN L-Phenylalanine, N-(N-acetyl-L-α-aspartyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L23 ANSWER 15 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:166121 HCAPLUS Full-text
DOCUMENT NUMBER: 108:166121
TITLE: Protease-catalyzed preparation of N-protected peptides
INVENTOR(S): Honda, Yutaka; Tsuchiya, Toyohito; Takemoto, Tadashi; Yugawa, Toshihide
PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

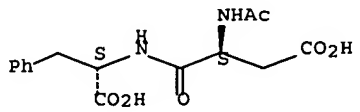
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62259597	A	19871111	JP 1986-104319	

198605
07

JP 06034745 B 19940511
PRIORITY APPLN. INFO.: JP 1986-104319
198605
07

ED Entered STN: 13 May 1988
AB N-Protected peptides or their derivs. were prepared by treating N-protected amino acids or their derivs. with amino acids or their derivs. in H2O of a two-phase medium composed of H2O containing protease and H2O-immiscible organic solvents containing quaternary ammonium or phosphonium salts and then transferring the resulting N-protected peptides containing ≥1 carboxyl group into the organic layer by forming ammonium or phosphonium salts, or by treating N-protected amino acids or their derivs. with amino acids or their derivs. in the presence of protease in H2O followed by extraction of the resulting N-protected peptides (containing ≥1 carboxyl group) with H2O-immiscible organic solvents containing quaternary ammonium salts or phosphonium salts. The method prevented products from hydrolysis with protease. Thus, protease M was dissolved in an aqueous solution of N-acetyl-L-aspartic acid and L-phenylalanine (I), and the solution was mixed with toluene containing trioctylmethylammonium chloride, and shaken at 40° for 24 h to give 4.2% (based on I; 1.2% from H2O layer and 3.0% from organic layer) Ac-Asp-Phe, vs. 1.6% for a reaction without addition of an organic solvent.
IT 108274-49-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by protease-catalyzed condensation of N-protected amino acids with amino acids)
RN 108274-49-3 HCAPLUS
CN L-Phenylalanine, N-(N-acetyl-L-α-aspartyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L23 ANSWER 16 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1987:214403 HCAPLUS Full-text
DOCUMENT NUMBER: 106:214403
TITLE: N-protected L-α-aspartyl-L-phenylalanine
INVENTOR(S): Takemoto, Tadashi; Yugawa, Toshihide; Hisamitsu, Kunio
PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62004299	A	19870110	JP 1985-144137	198507 01
JP 06080074	B	19941012		
CA 1274950	A1	19901002	CA 1986-512467	198606 26

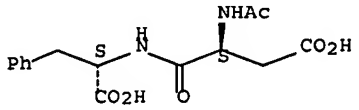
US 4740616	A	19880426	US 1986-883354	198607 01
US 4789758	A	19881206	US 1987-106801	198710 13
JP 07070177	A	19950314	JP 1994-70542	199404 08
JP 2513155	B2	19960703		

PRIORITY APPLN. INFO.:

JP 1985-144137	A	198507 01
US 1986-872020	A2	198606 09
US 1986-883354	A3	198607 01

OTHER SOURCE(S): CASREACT 106:214403
ED Entered STN: 26 Jun 1987
AB Title compds., useful as intermediates for aspartame, were prepared by treating N-protected L-aspartic anhydride with alkali metal salts, alkaline earth metal salts, or organic amine salts of L-phenylalanine in aqueous media. Thus, N-formyl-L-aspartic anhydride was added to an aqueous solution of L-PhCH2CH(NH2)CO2Na.H2O at pH 12.0-12.5 and 5° in 1 h to give 68.2% N-formyl-L-β-aspartyl-L-phenylalanine.
IT 108274-49-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for aspartame)
RN 108274-49-3 HCAPLUS
CN L-Phenylalanine, N-(N-acetyl-L-α-aspartyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L23 ANSWER 17 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:168847 HCAPLUS Full-text
DOCUMENT NUMBER: 104:168847
TITLE: Dipeptide derivatives
PATENT ASSIGNEE(S): Flork, Michel, Fr.
SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 60042396	A	19850306	JP 1983-150112	198308 17

PRIORITY APPLN. INFO.:

JP 1983-150112	198308

ED Entered STN: 17 May 1986

AB The title compds., useful as central nervous system agents (no data), were prepared Thus, 240 g (N-acetylasparaginimido)glutamic acid was added to a mixture of 198 g (3,4-dihydroxyphenyl)alanine and 1 mL H2O at 0° and pH 8.5 (digested with the addition of 5 N NaOH) and the resulting mixture eluted over Duolite and the eluant acidified with HCl and then heated at 45° for 1 h to give N-acetyl-α-aspartyl-α-glutamyl-(3,4-dihydroxyphenyl)alanine.

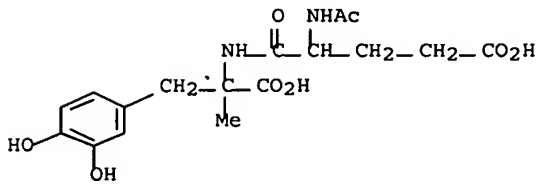
IT 101679-23-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of, as central nervous system agent)

RN 101679-23-6 HCAPLUS

CN Tyrosine, N-(N-acetyl-L-α-glutamyl)-3-hydroxy-α-methyl- (9CI) (CA INDEX NAME)



L23 ANSWER 18 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1985:422916 HCAPLUS Full-text

DOCUMENT NUMBER: 103:22916

TITLE: Specific cleavage of peptides containing an aspartic acid (β-hydroxamic acid) residue

AUTHOR(S): Blodgett, James K.; Loudon, G. Marc; Collins, Kim D.

CORPORATE SOURCE: Sch. Pharm. Pharm. Sci., Purdue Univ., West Lafayette, IN, 47907, USA

SOURCE: Journal of the American Chemical Society (1985), 107(14), 4305-13
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 27 Jul 1985

AB Peptides containing the aspartyl β-hydroxamic acid residues are cleaved specifically at the carboxyl side of this residue at pH ≥6. The cleavage occurs by attack of both the hydroxamic acid nitrogen and the hydroxamic acid oxygen to yield tetrahedral intermediates that, in the rate-limiting step, break down with cleavage of the peptide chain. In a competing reaction, the peptide nitrogen on the carboxyl side attacks the hydroxamate carbonyl to expel hydroxylamine and give an imide intermediate. The cleavage yield reflects the relative efficiency of these two pathways. The extent of cleavage is dramatically increased in the presence of 1 M hydroxylamine. The extent of cleavage is also increased significantly by phosphate buffers, but not by PIPES or imidazole buffers, in the absence of added hydroxylamine. The role of hydroxylamine in some cases may be to intercept the imide or the isoimide; but in at least two cases evidence is presented that hydroxylamine, like phosphate, may be acting as a general acid-base catalyst that selectively catalyzes the breakdown of tetrahedral intermediates leading to chain cleavage. Peptides containing glutamyl (γ-hydroxamic acid) residues are also cleaved, but at rates that are 20-40 times slower than those of the analogous aspartyl peptides.

IT 96363-02-9

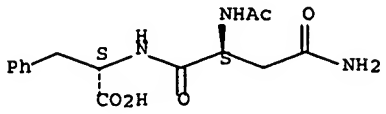
RL: RCT (Reactant); RACT (Reactant or reagent)

(specific cleavage of)

RN 96363-02-9 HCAPLUS

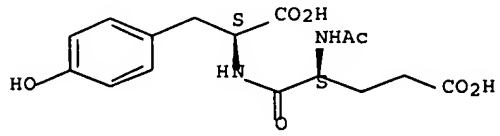
CN L-Phenylalanine, N-(N2-acetyl-L-asparaginyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L23 ANSWER 19 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1979:138176 HCAPLUS Full-text
DOCUMENT NUMBER: 90:138176
TITLE: Reduction of oligopeptides to amino alcohols with borane
AUTHOR(S): Frank, Hartmut; Desiderio, Dominic M.
CORPORATE SOURCE: Inst. Lipid Res., Baylor Coll. Med., Houston, TX, USA
SOURCE: Analytical Biochemistry (1978), 90(1), 413-19
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
AB Oligopeptides were reduced with 1M borane in THF at 90° for 30 min to give amino alcs., which were analyzed by thin-layer and gas chromatog. and mass spectrometry. This borane reduction did not give the side products which are formed by LiAlH4 reduction Borane reduction can be used in the separation and identification of constituents of oligopeptide mixts. by gas chromatog.-mass spectrometry during peptide sequencing.
IT 69624-05-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, by borane, amino alcs. from)
RN 69624-05-1 HCAPLUS
CN L-Tyrosine, N-(N-acetyl-L-α-glutamyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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